

Sample name: **M18_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric Result

logP (XH2 +) -0.21 ±0.12 (n=50)
 logP (neutral XH) 2.63 ±0.02 (n=50)
 logP (X -) 0.46
 RMSD 0.583

18C-09016 Points 2 to 28

M18_octanol concentration factor 1.091
 Carbonate 0.1016 mM
 Acidity error -0.00215 mM

18C-09016 Points 29 to 56

M18_octanol concentration factor 1.051
 Carbonate 0.0884 mM
 Acidity error -0.10411 mM

18C-09016 Points 57 to 86

M18_octanol concentration factor 1.063
 Carbonate 0.1449 mM
 Acidity error 0.00187 mM

Warnings and errors

Errors None
 Warnings None

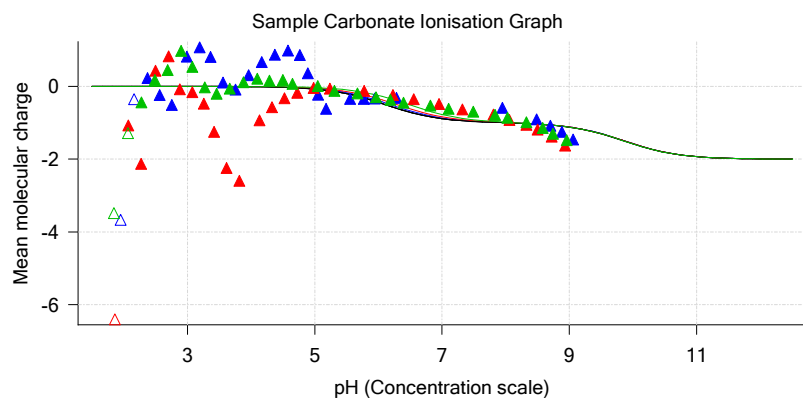
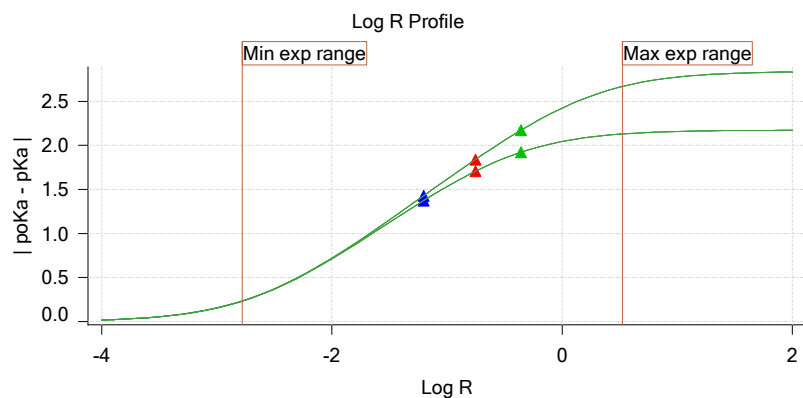
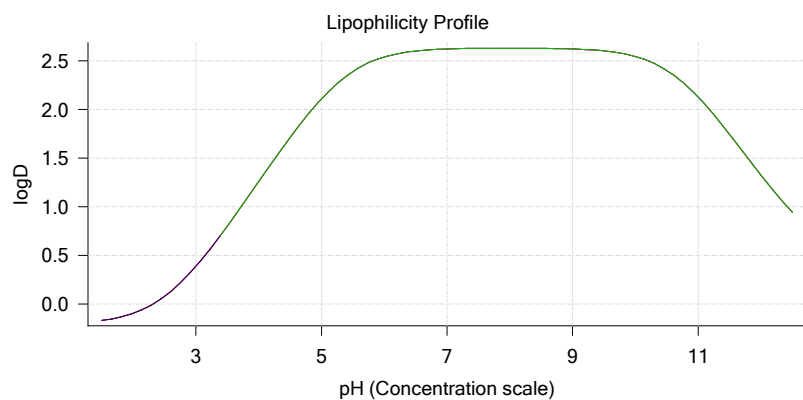
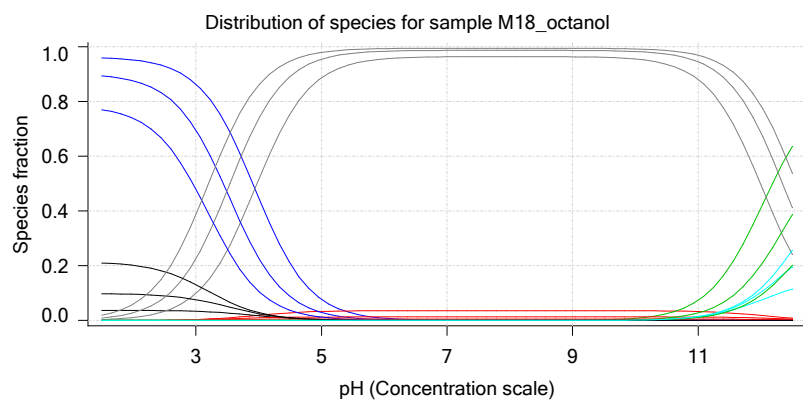
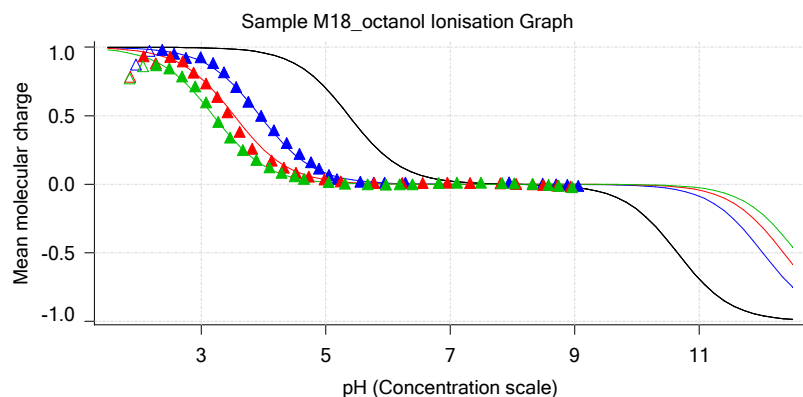
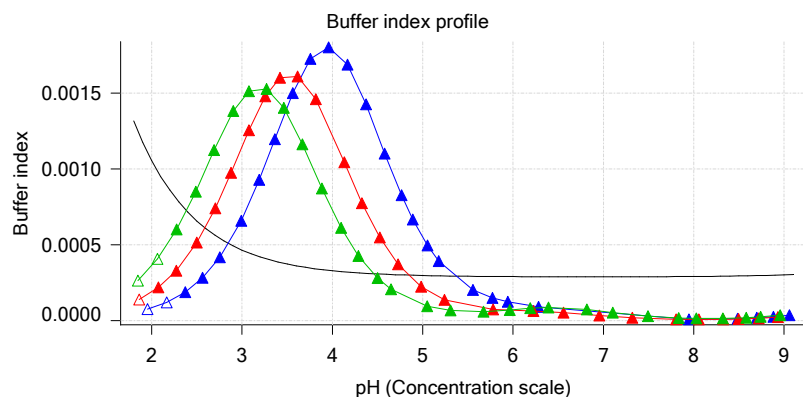
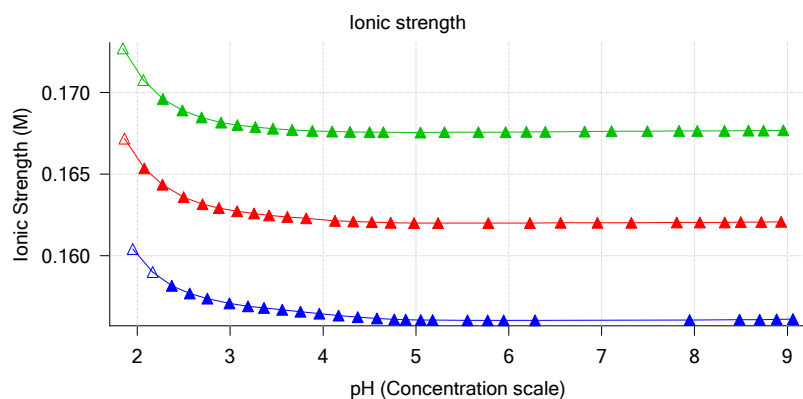
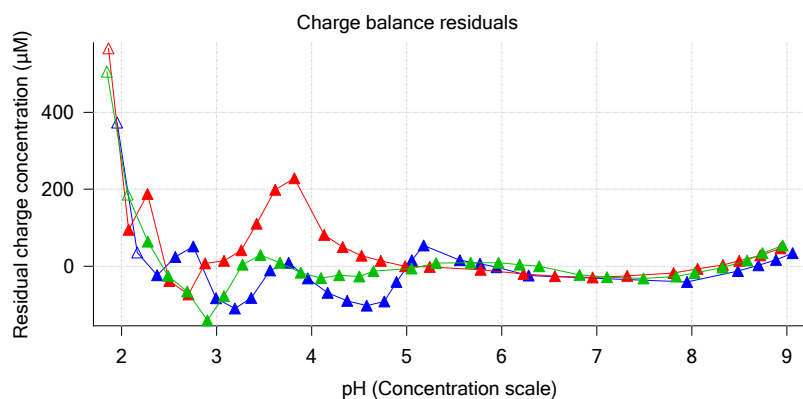
Sample logD and percent species

pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-0.19	61.03 %	0.00 %	0.00 %	37.85 %	1.12 %	0.00 %	Stomach pH
1.200	-0.19	60.63 %	0.00 %	0.00 %	37.60 %	1.76 %	0.00 %	
2.000	-0.10	55.44 %	0.02 %	0.00 %	34.39 %	10.15 %	0.00 %	
3.000	0.39	28.95 %	0.12 %	0.00 %	17.95 %	52.98 %	0.00 %	Blood pH
4.000	1.26	5.01 %	0.21 %	0.00 %	3.11 %	91.67 %	0.00 %	
5.000	2.11	0.54 %	0.23 %	0.00 %	0.34 %	98.89 %	0.00 %	
6.000	2.54	0.05 %	0.23 %	0.00 %	0.03 %	99.68 %	0.00 %	
6.500	2.60	0.02 %	0.23 %	0.00 %	0.01 %	99.74 %	0.00 %	
7.000	2.62	0.01 %	0.23 %	0.00 %	0.00 %	99.76 %	0.00 %	
7.400	2.63	0.00 %	0.23 %	0.00 %	0.00 %	99.76 %	0.00 %	
8.000	2.63	0.00 %	0.23 %	0.00 %	0.00 %	99.76 %	0.00 %	
9.000	2.62	0.00 %	0.23 %	0.01 %	0.00 %	99.75 %	0.02 %	
10.000	2.55	0.00 %	0.23 %	0.05 %	0.00 %	99.57 %	0.15 %	
11.000	2.13	0.00 %	0.23 %	0.51 %	0.00 %	97.79 %	1.47 %	
12.000	1.32	0.00 %	0.19 %	4.33 %	0.00 %	82.99 %	12.49 %	

Sample name: **M18_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

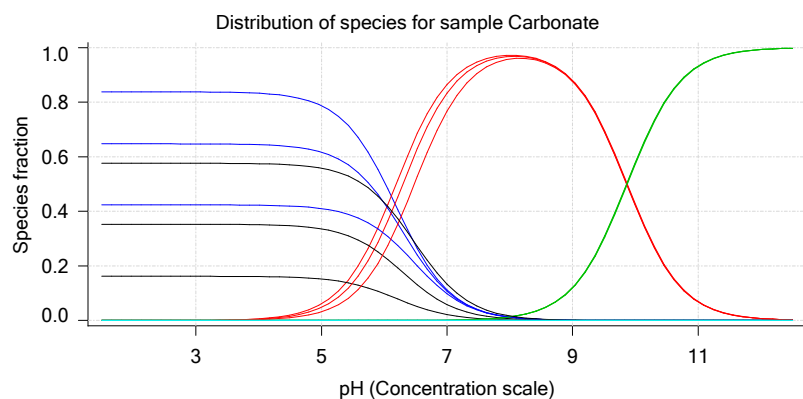
Graphs



Sample name: **M18_octanol**
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Graphs (continued)



Sample name: **M18_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-09016 Points 2 to 28

Overall results

RMSD 0.731
 Average ionic strength 0.156 M
 Average temperature 24.9°C
 Partition ratio 0.0626 : 1
 Analyte concentration range 2691.8 µM to 2763.3 µM
 Total points considered 25 of 27

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.102 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 S 0.9967 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 jH 1.2 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 jOH 0.0 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r

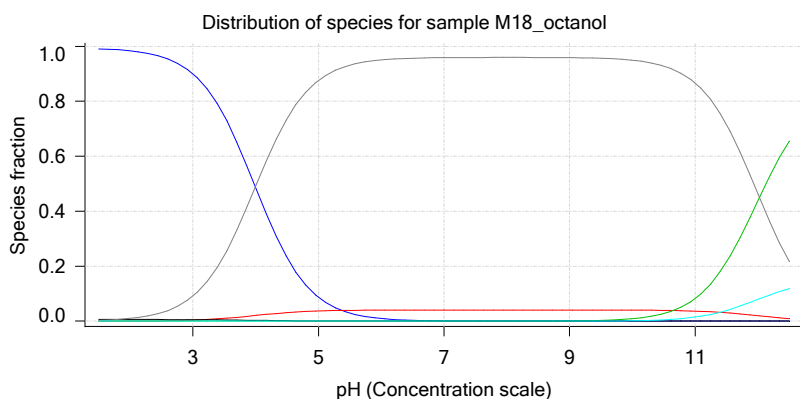
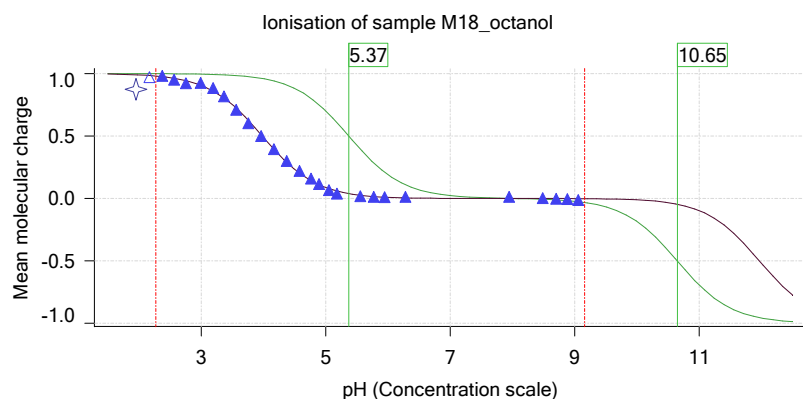
Titrants

0.50 M HCl 0.999843 3/9/2018 11:02:44 PM C:\Sirius_T3\HCl18C09.t3r
 0.50 M KOH 0.999845 3/9/2018 11:02:44 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor 1.091
 Base pKa 1 5.37
 Acid pKa 2 10.65
 logP (XH₂⁺) -1.02
 logP (neutral XH) 2.58
 logP (X⁻) 0.46

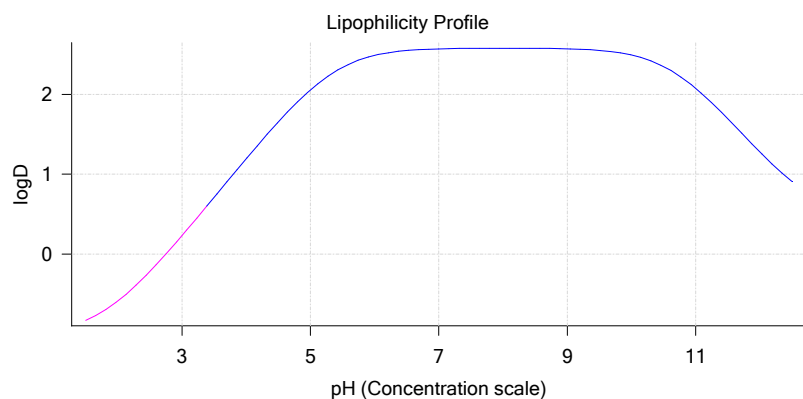
Sample graphs



Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09016**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



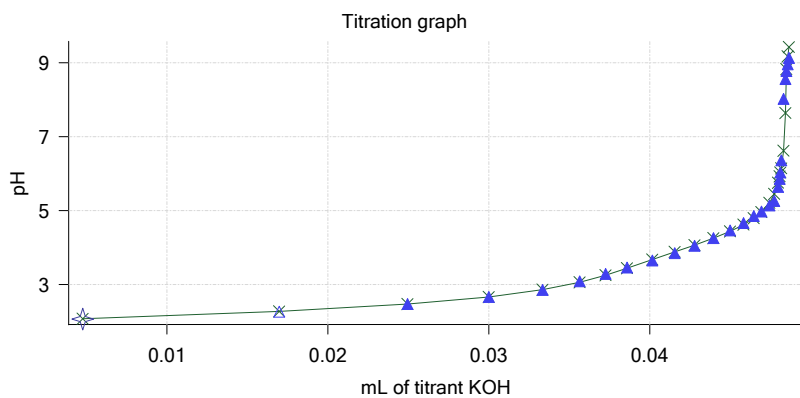
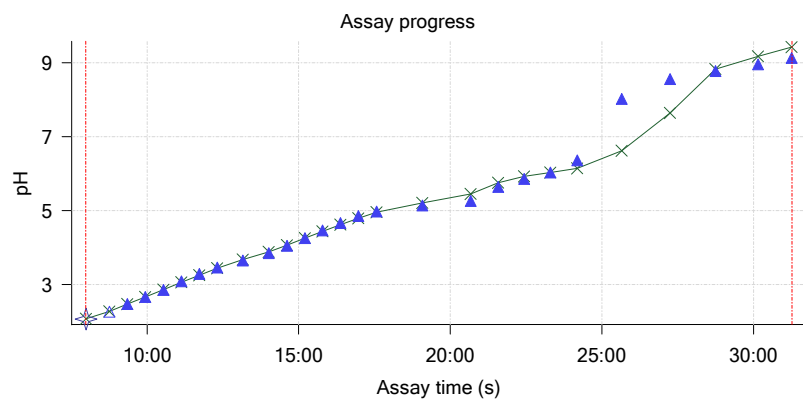
Sample logD and percent species

pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-0.95	99.30 %	0.00 %	0.00 %	0.60 %	0.10 %	0.00 %	Stomach pH
1.200	-0.91	99.24 %	0.01 %	0.00 %	0.60 %	0.16 %	0.00 %	
2.000	-0.59	98.37 %	0.04 %	0.00 %	0.59 %	1.00 %	0.00 %	
3.000	0.23	89.97 %	0.38 %	0.00 %	0.54 %	9.11 %	0.00 %	
4.000	1.19	48.52 %	2.07 %	0.00 %	0.29 %	49.12 %	0.00 %	Blood pH
5.000	2.06	8.65 %	3.69 %	0.00 %	0.05 %	87.60 %	0.00 %	
6.000	2.49	0.94 %	4.00 %	0.00 %	0.01 %	95.05 %	0.00 %	
6.500	2.55	0.30 %	4.03 %	0.00 %	0.00 %	95.67 %	0.00 %	
7.000	2.57	0.09 %	4.04 %	0.00 %	0.00 %	95.86 %	0.00 %	
7.400	2.57	0.04 %	4.04 %	0.00 %	0.00 %	95.92 %	0.00 %	
8.000	2.58	0.01 %	4.04 %	0.01 %	0.00 %	95.94 %	0.00 %	
9.000	2.57	0.00 %	4.04 %	0.09 %	0.00 %	95.85 %	0.02 %	
10.000	2.49	0.00 %	4.00 %	0.90 %	0.00 %	94.94 %	0.16 %	
11.000	2.08	0.00 %	3.65 %	8.18 %	0.00 %	86.70 %	1.48 %	
12.000	1.28	0.00 %	1.95 %	43.76 %	0.00 %	46.39 %	7.90 %	

Carbonate and acidity

Carbonate 0.102 mM
Acidity error -0.002 mM

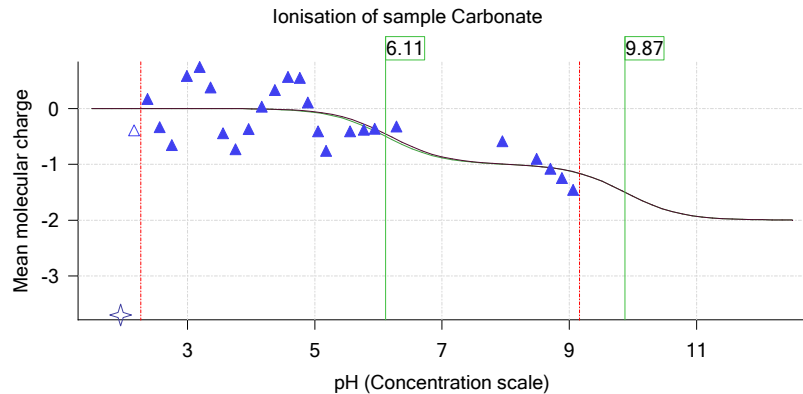
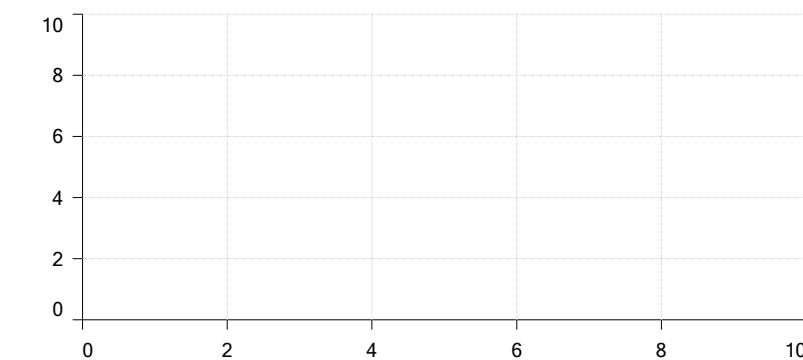
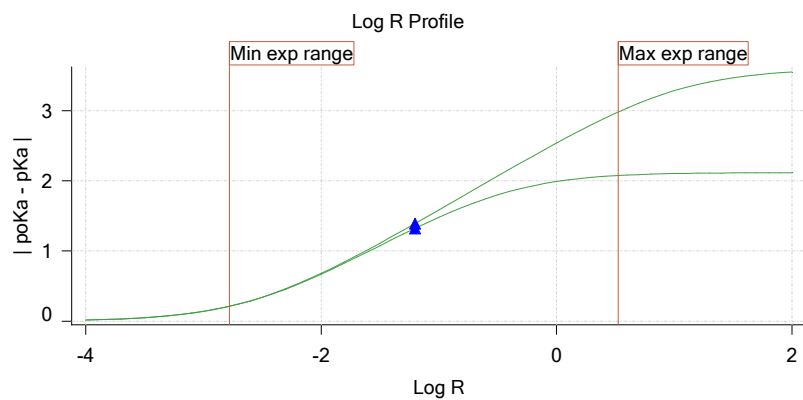
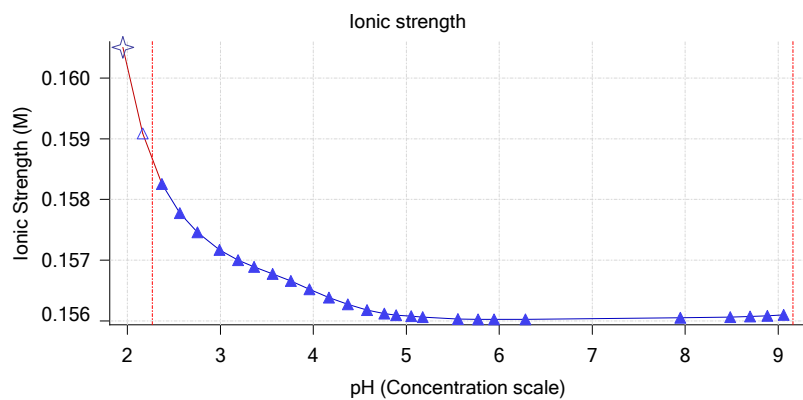
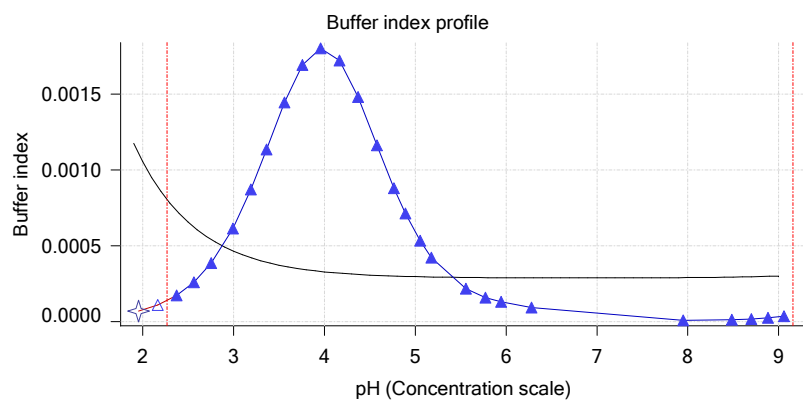
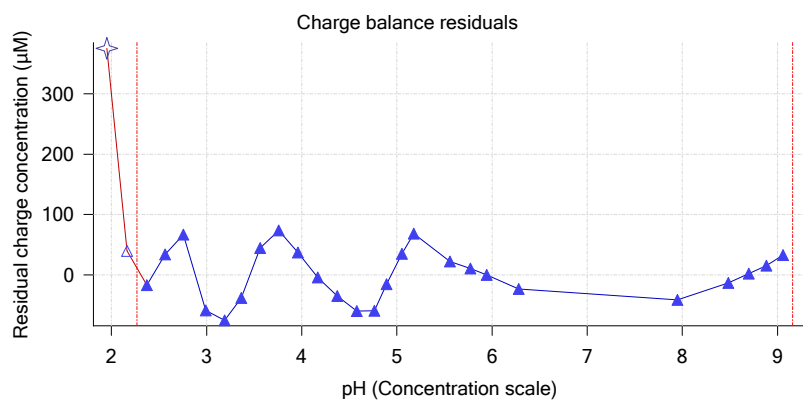
Other graphs



Sample name: **M18_octanol**
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 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

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 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



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 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-09016 Points 29 to 56

Overall results

RMSD 0.550
 Average ionic strength 0.162 M
 Average temperature 25.0°C
 Partition ratio 0.1763 : 1
 Analyte concentration range 2278.7 µM to 2341.3 µM
 Total points considered 27 of 28

Warnings and errors

Errors None
 Warnings One or more logP values out of range

Four-Plus parameters

Alpha 0.102 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 S 0.9967 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 jH 1.2 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 jOH 0.0 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r

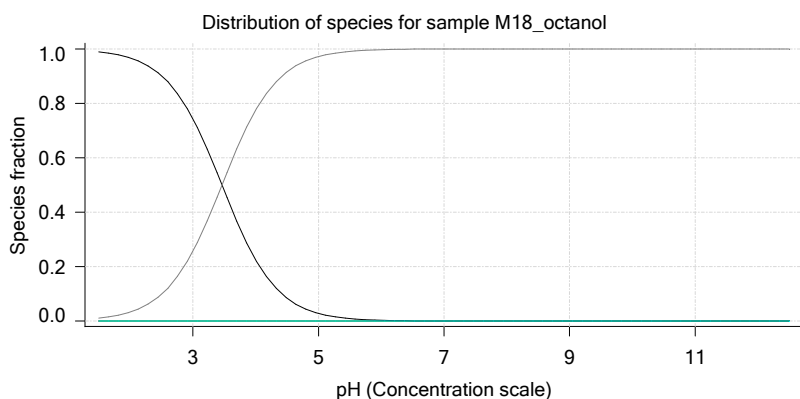
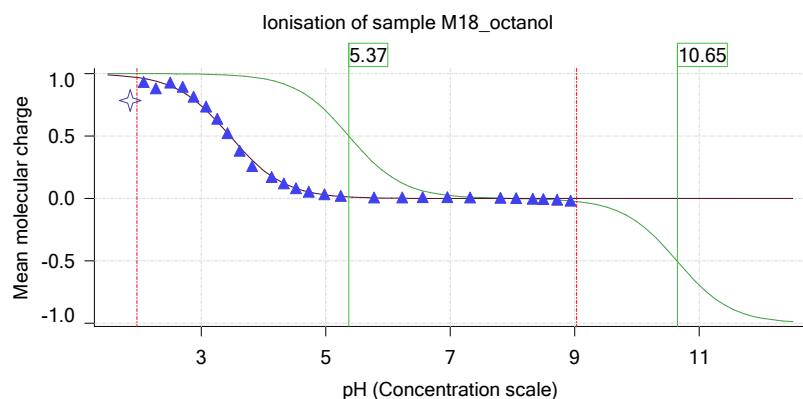
Titrants

0.50 M HCl 0.999843 3/9/2018 11:02:44 PM C:\Sirius_T3\HCl18C09.t3r
 0.50 M KOH 0.999845 3/9/2018 11:02:44 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor 1.051
 Base pKa 1 5.37
 Acid pKa 2 10.65
 logP (XH₂⁺) 7.44
 logP (neutral XH) 9.35
 logP (X⁻) 0.46

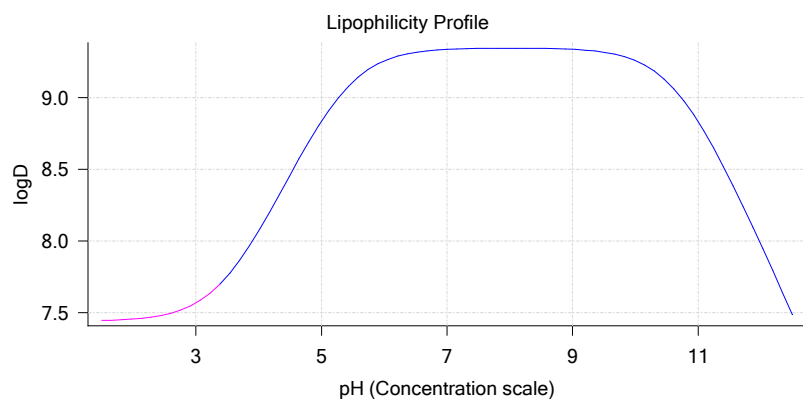
Sample graphs



Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09016**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



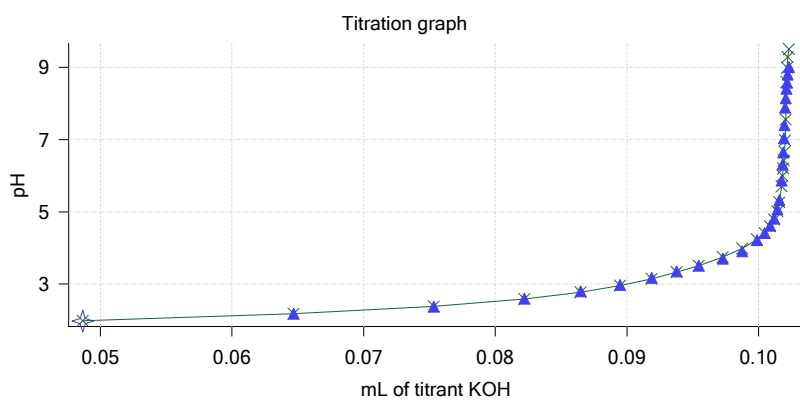
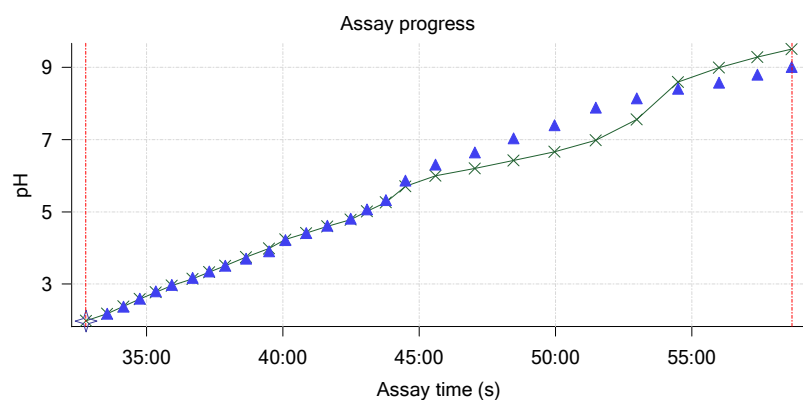
Sample logD and percent species

pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	7.44	0.00 %	0.00 %	0.00 %	99.66 %	0.34 %	0.00 %	Stomach pH
1.200	7.44	0.00 %	0.00 %	0.00 %	99.46 %	0.54 %	0.00 %	
2.000	7.45	0.00 %	0.00 %	0.00 %	96.66 %	3.34 %	0.00 %	
3.000	7.57	0.00 %	0.00 %	0.00 %	74.32 %	25.68 %	0.00 %	
4.000	8.07	0.00 %	0.00 %	0.00 %	22.45 %	77.55 %	0.00 %	Blood pH
5.000	8.84	0.00 %	0.00 %	0.00 %	2.81 %	97.19 %	0.00 %	
6.000	9.26	0.00 %	0.00 %	0.00 %	0.29 %	99.71 %	0.00 %	
6.500	9.32	0.00 %	0.00 %	0.00 %	0.09 %	99.91 %	0.00 %	
7.000	9.34	0.00 %	0.00 %	0.00 %	0.03 %	99.97 %	0.00 %	
7.400	9.34	0.00 %	0.00 %	0.00 %	0.01 %	99.99 %	0.00 %	
8.000	9.35	0.00 %	0.00 %	0.00 %	0.00 %	100.00 %	0.00 %	
9.000	9.34	0.00 %	0.00 %	0.00 %	0.00 %	100.00 %	0.00 %	
10.000	9.26	0.00 %	0.00 %	0.00 %	0.00 %	100.00 %	0.00 %	
11.000	8.84	0.00 %	0.00 %	0.00 %	0.00 %	100.00 %	0.00 %	
12.000	7.98	0.00 %	0.00 %	0.00 %	0.00 %	100.00 %	0.00 %	

Carbonate and acidity

Carbonate 0.088 mM
Acidity error -0.104 mM

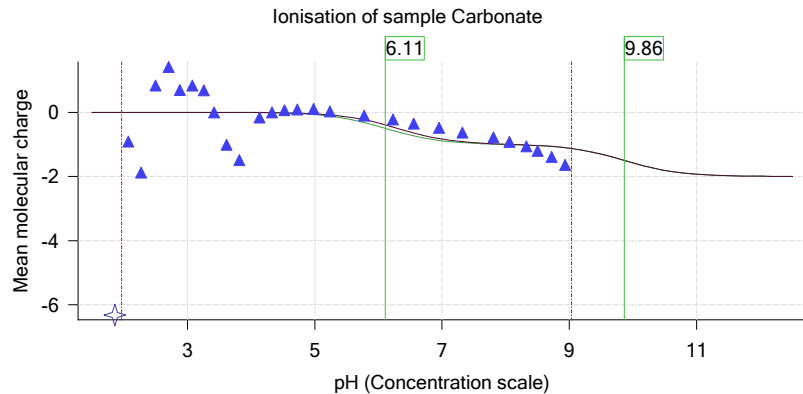
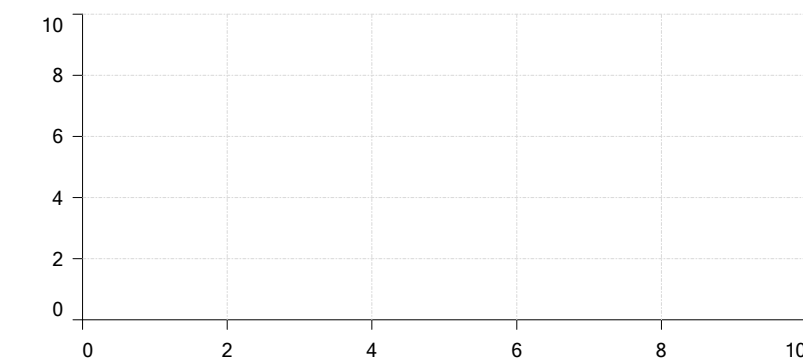
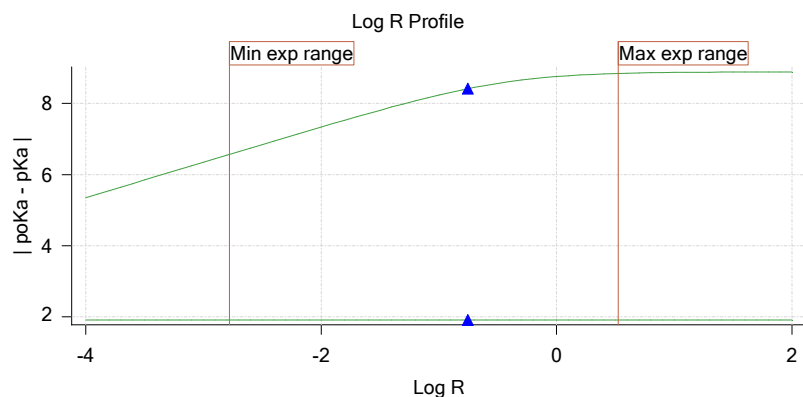
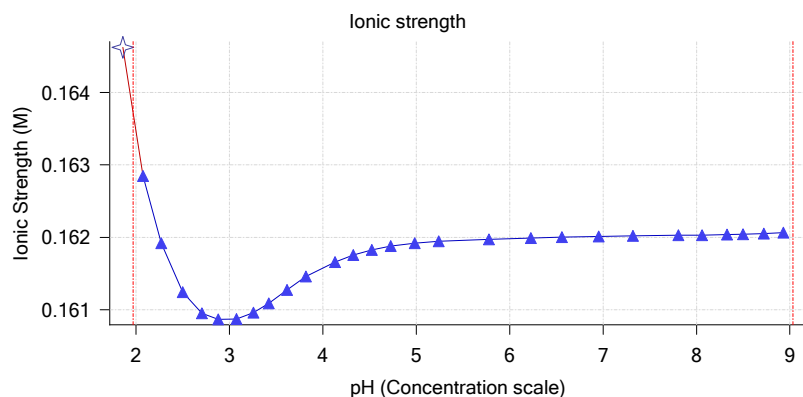
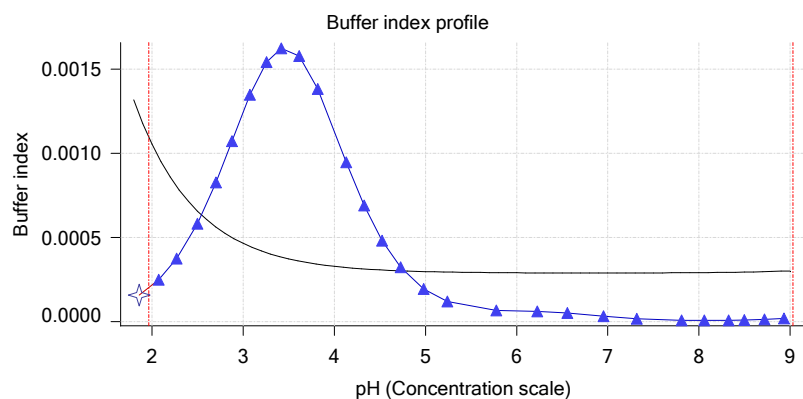
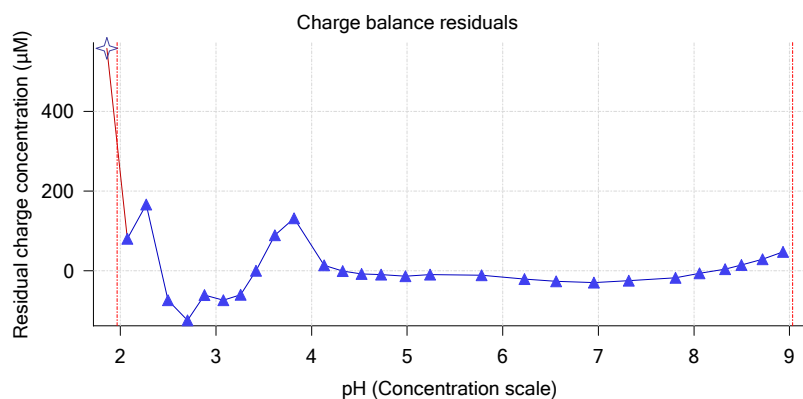
Other graphs



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Other graphs (continued)



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 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-09016 Points 57 to 86

Overall results

RMSD 0.447
 Average ionic strength 0.168 M
 Average temperature 25.0°C
 Partition ratio 0.4400 : 1
 Analyte concentration range 1742.6 µM to 1782.5 µM
 Total points considered 28 of 30

Warnings and errors

Errors None
 Warnings One or more logP values out of range

Four-Plus parameters

Alpha 0.102 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 S 0.9967 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 jH 1.2 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r
 jOH 0.0 3/9/2018 11:02:43 PM C:\Sirius_T3\HCl18C09.t3r

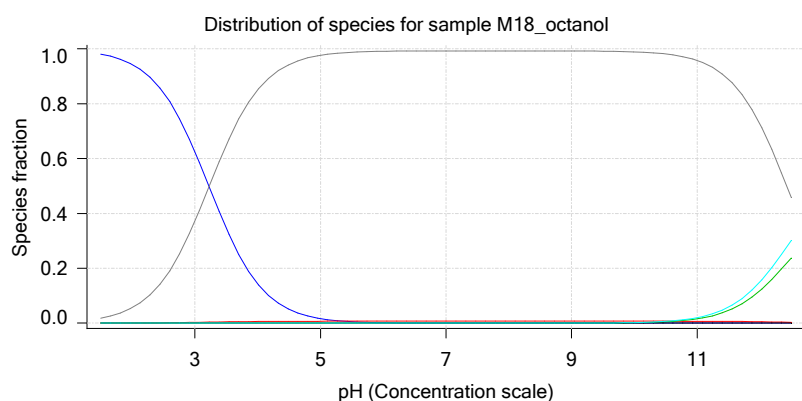
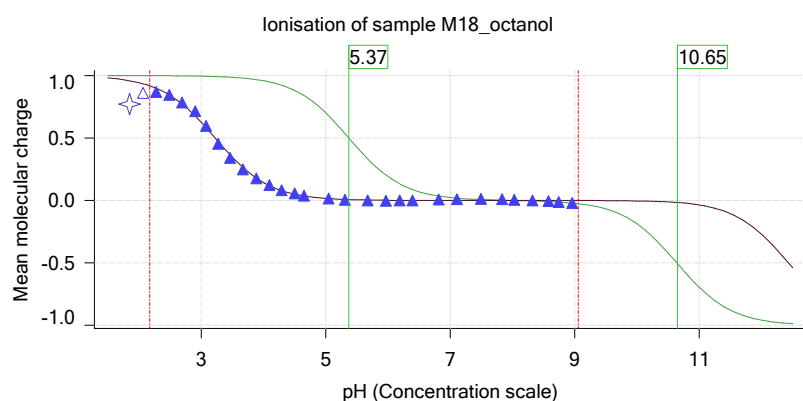
Titrants

0.50 M HCl 0.999843 3/9/2018 11:02:44 PM C:\Sirius_T3\HCl18C09.t3r
 0.50 M KOH 0.999845 3/9/2018 11:02:44 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor 1.063
 Base pKa 1 5.37
 Acid pKa 2 10.65
 logP (XH₂⁺) -3.10
 logP (neutral XH) 2.50
 logP (X⁻) 0.46

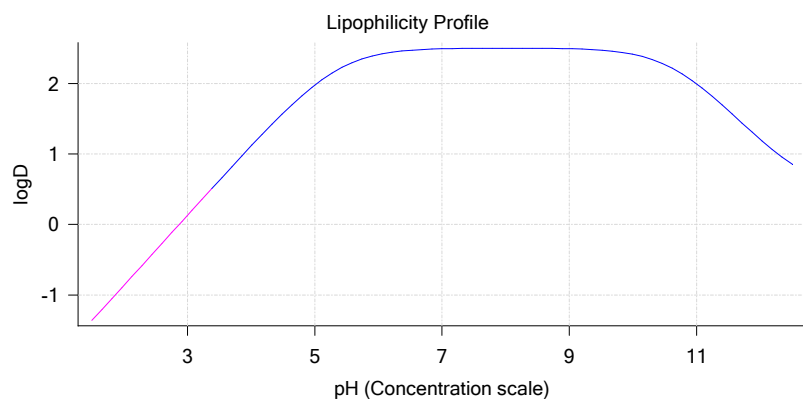
Sample graphs



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Sample graphs (continued)



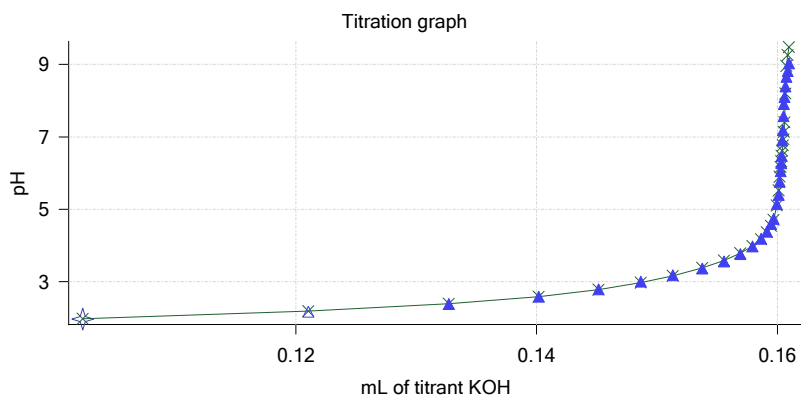
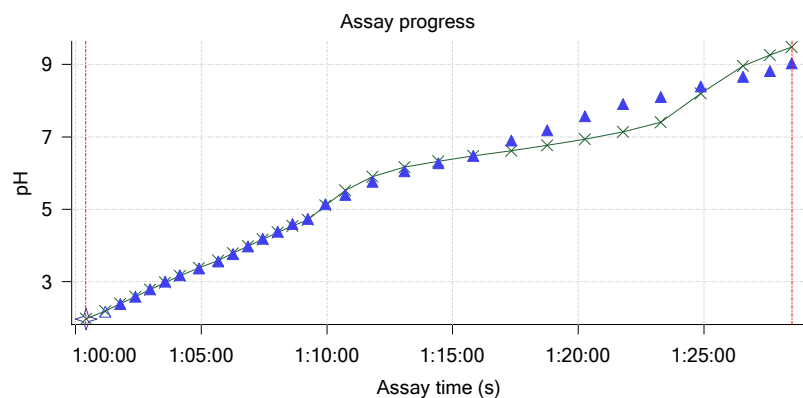
Sample logD and percent species

pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-1.84	99.37 %	0.00 %	0.00 %	0.04 %	0.59 %	0.00 %	Stomach pH
1.200	-1.65	99.02 %	0.01 %	0.00 %	0.03 %	0.94 %	0.00 %	
2.000	-0.87	94.30 %	0.04 %	0.00 %	0.03 %	5.63 %	0.00 %	
3.000	0.13	62.45 %	0.27 %	0.00 %	0.02 %	37.26 %	0.00 %	
4.000	1.11	14.26 %	0.61 %	0.00 %	0.01 %	85.12 %	0.00 %	Blood pH
5.000	1.98	1.64 %	0.70 %	0.00 %	0.00 %	97.66 %	0.00 %	
6.000	2.41	0.17 %	0.71 %	0.00 %	0.00 %	99.13 %	0.00 %	
6.500	2.47	0.05 %	0.71 %	0.00 %	0.00 %	99.24 %	0.00 %	
7.000	2.49	0.02 %	0.71 %	0.00 %	0.00 %	99.27 %	0.00 %	
7.400	2.50	0.01 %	0.71 %	0.00 %	0.00 %	99.28 %	0.00 %	
8.000	2.50	0.00 %	0.71 %	0.00 %	0.00 %	99.28 %	0.00 %	
9.000	2.49	0.00 %	0.71 %	0.02 %	0.00 %	99.25 %	0.02 %	
10.000	2.42	0.00 %	0.71 %	0.16 %	0.00 %	98.93 %	0.20 %	
11.000	2.00	0.00 %	0.69 %	1.53 %	0.00 %	95.84 %	1.95 %	
12.000	1.21	0.00 %	0.52 %	11.68 %	0.00 %	72.98 %	14.82 %	

Carbonate and acidity

Carbonate 0.145 mM
 Acidity error 0.002 mM

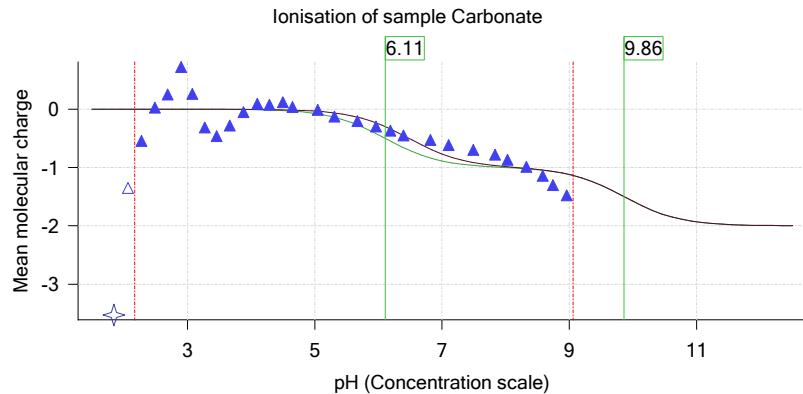
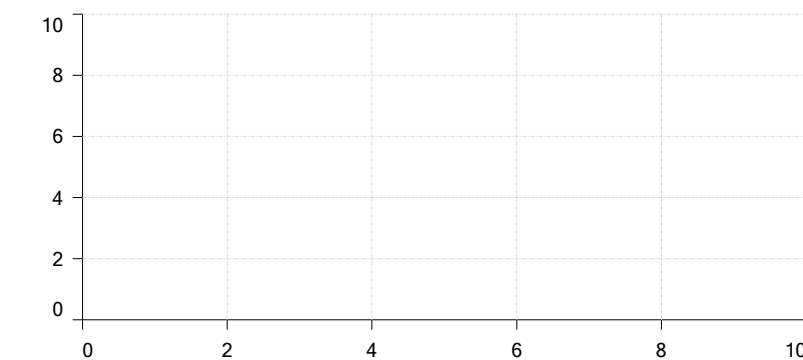
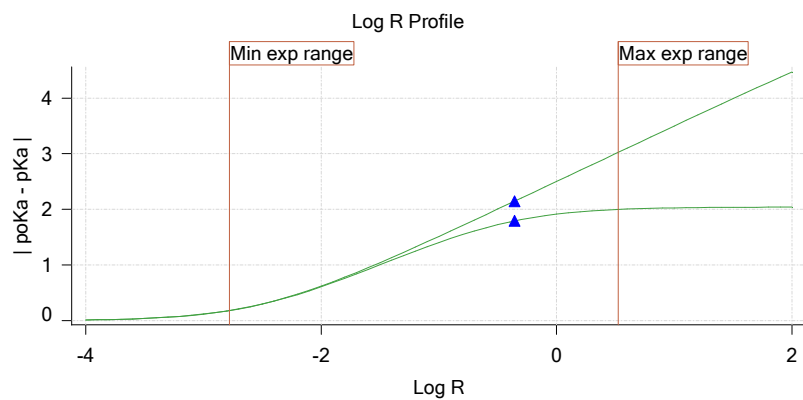
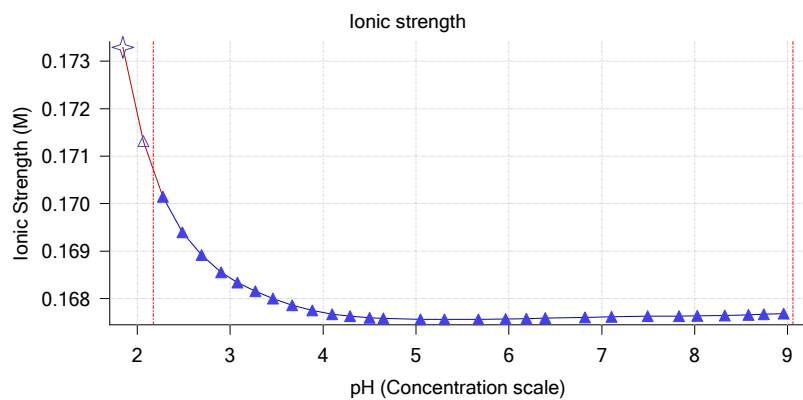
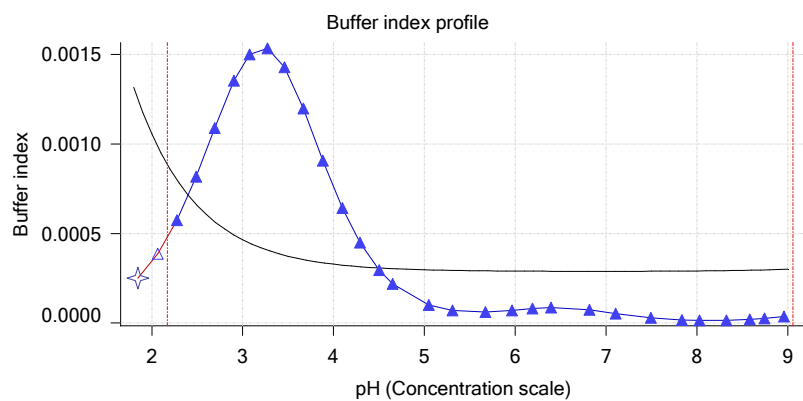
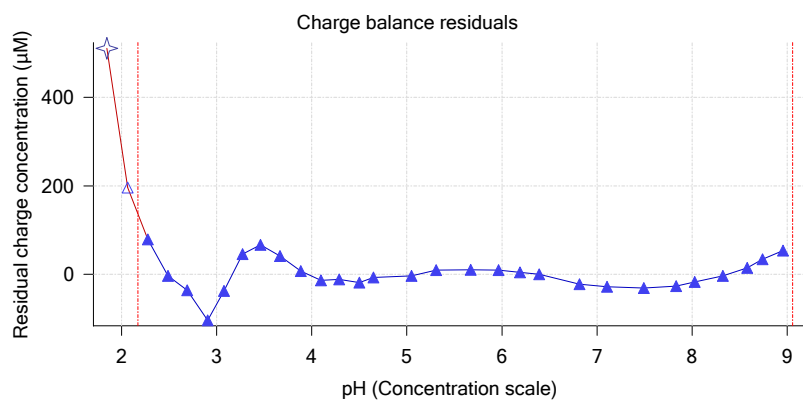
Other graphs



Sample name: **M18_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)





Assay model

Sample name: **M18_octanol** Experiment start time: **3/9/2018 11:02:44 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-09016** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M18_octanol	2/27/2018 7:08:39 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001220 g	3/9/2018 2:22:52 PM	User entered value
Formula weight	267.11 g/mol	2/27/2018 7:08:39 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	267.11	2/27/2018 7:08:39 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 7:08:39 PM	User entered value
Sample is a	Ampholyte	2/27/2018 7:08:39 PM	User entered value
pKa 1	5.37	2/27/2018 7:08:39 PM	User entered value
Type	Base	2/27/2018 7:08:39 PM	User entered value
pKa 2	10.65	2/27/2018 7:08:39 PM	User entered value
Type	Acid	2/27/2018 7:08:39 PM	User entered value
logp (XH ₂ +)	-0.35	2/28/2018 3:20:28 PM	User entered value
logP (neutral XH)	2.57	3/2/2018 4:34:50 PM	User entered value
logP (X -)	0.46	2/27/2018 7:09:34 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/ time
4:58.7	Manual volume addition				0.10000 mL					
4:59.8	Initial pH = 7.99									
7:59.3	Data point 2	1.50000 mL	0.04812 mL	0.00477 mL	0.10000 mL	2.062	-0.00681	0.27502	0.00064	10.0 s
8:45.5	Data point 3	1.50000 mL	0.04812 mL	0.01698 mL	0.10000 mL	2.268	0.00821	0.44883	0.00061	10.0 s
9:21.1	Data point 4	1.50000 mL	0.04812 mL	0.02495 mL	0.10000 mL	2.471	-0.00977	0.70424	0.00058	10.0 s
9:56.6	Data point 5	1.50000 mL	0.04812 mL	0.03001 mL	0.10000 mL	2.662	-0.00069	0.07464	0.00012	10.0 s
10:32.1	Data point 6	1.50000 mL	0.04812 mL	0.03335 mL	0.10000 mL	2.850	-0.00288	0.33859	0.00024	10.0 s
11:07.6	Data point 7	1.50000 mL	0.04812 mL	0.03565 mL	0.10000 mL	3.085	-0.01383	0.83922	0.00074	10.0 s
11:43.3	Data point 8	1.50000 mL	0.04812 mL	0.03725 mL	0.10000 mL	3.283	-0.00418	0.74326	0.00024	10.0 s
12:18.8	Data point 9	1.50000 mL	0.04812 mL	0.03859 mL	0.10000 mL	3.456	-0.01450	0.85812	0.00077	10.0 s
13:09.7	Data point 10	1.50000 mL	0.04812 mL	0.04017 mL	0.10000 mL	3.653	-0.01030	0.40559	0.00080	10.0 s
14:00.8	Data point 11	1.50000 mL	0.04812 mL	0.04156 mL	0.10000 mL	3.848	-0.00945	0.70466	0.00056	10.5 s
14:36.7	Data point 12	1.50000 mL	0.04812 mL	0.04278 mL	0.10000 mL	4.049	-0.00976	0.86426	0.00052	10.0 s
15:12.1	Data point 13	1.50000 mL	0.04812 mL	0.04396 mL	0.10000 mL	4.256	-0.00996	0.79638	0.00055	10.0 s
15:47.4	Data point 14	1.50000 mL	0.04812 mL	0.04499 mL	0.10000 mL	4.460	-0.01429	0.84980	0.00077	10.0 s
16:22.8	Data point 15	1.50000 mL	0.04812 mL	0.04584 mL	0.10000 mL	4.667	-0.01676	0.72668	0.00097	10.0 s
16:58.2	Data point 16	1.50000 mL	0.04812 mL	0.04647 mL	0.10000 mL	4.852	-0.01624	0.82288	0.00088	10.5 s
17:34.1	Data point 17	1.50000 mL	0.04812 mL	0.04694 mL	0.10000 mL	4.977	-0.06194	0.99731	0.00306	Time out at

Sample name: **M18_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
19:04.6	Data point 18	1.50000 mL	0.04812 mL	0.04744 mL	0.10000 mL	5.138	-0.02805	0.99638	0.00139	Timed out at 59.5 s
20:40.3	Data point 19	1.50000 mL	0.04812 mL	0.04774 mL	0.10000 mL	5.264	-0.01845	0.96248	0.00093	29.0 s
21:34.7	Data point 20	1.50000 mL	0.04812 mL	0.04798 mL	0.10000 mL	5.641	-0.01992	0.97402	0.00100	21.0 s
22:26.3	Data point 21	1.50000 mL	0.04812 mL	0.04807 mL	0.10000 mL	5.855	-0.01912	0.93098	0.00098	26.5 s
23:18.2	Data point 22	1.50000 mL	0.04812 mL	0.04812 mL	0.10000 mL	6.027	-0.01851	0.97469	0.00093	27.5 s
24:11.1	Data point 23	1.50000 mL	0.04812 mL	0.04817 mL	0.10000 mL	6.363	-0.01958	0.96477	0.00099	57.5 s
25:39.1	Data point 24	1.50000 mL	0.04812 mL	0.04831 mL	0.10000 mL	8.024	-0.07733	0.99662	0.00383	Timed out at 59.5 s
27:14.7	Data point 25	1.50000 mL	0.04812 mL	0.04842 mL	0.10000 mL	8.560	-0.02632	0.98996	0.00131	Timed out at 59.5 s
28:45.1	Data point 26	1.50000 mL	0.04812 mL	0.04849 mL	0.10000 mL	8.774	-0.02007	0.98634	0.00100	48.0 s
30:08.9	Data point 27	1.50000 mL	0.04812 mL	0.04857 mL	0.10000 mL	8.957	-0.01923	0.96603	0.00097	36.0 s
31:15.5	Data point 28	1.50000 mL	0.04812 mL	0.04866 mL	0.10000 mL	9.132	-0.01929	0.95230	0.00098	29.0 s
32:47.3	Data point 29	1.50000 mL	0.10212 mL	0.04866 mL	0.30000 mL	1.972	0.00050	0.00545	0.00033	10.5 s
33:34.0	Data point 30	1.50000 mL	0.10212 mL	0.06468 mL	0.30000 mL	2.179	-0.01398	0.77392	0.00078	10.0 s
34:09.7	Data point 31	1.50000 mL	0.10212 mL	0.07533 mL	0.30000 mL	2.373	0.00146	0.41139	0.00011	10.0 s
34:45.3	Data point 32	1.50000 mL	0.10212 mL	0.08220 mL	0.30000 mL	2.598	-0.00003	0.00017	0.00012	10.0 s
35:20.8	Data point 33	1.50000 mL	0.10212 mL	0.08648 mL	0.30000 mL	2.799	-0.00882	0.36125	0.00072	10.0 s
35:56.2	Data point 34	1.50000 mL	0.10212 mL	0.08946 mL	0.30000 mL	2.973	-0.00669	0.54661	0.00045	10.0 s
36:42.0	Data point 35	1.50000 mL	0.10212 mL	0.09186 mL	0.30000 mL	3.170	-0.01175	0.75450	0.00067	10.5 s
37:18.0	Data point 36	1.50000 mL	0.10212 mL	0.09377 mL	0.30000 mL	3.350	-0.00456	0.45623	0.00033	10.0 s
37:53.4	Data point 37	1.50000 mL	0.10212 mL	0.09544 mL	0.30000 mL	3.512	-0.00080	0.01535	0.00032	10.0 s
38:39.1	Data point 38	1.50000 mL	0.10212 mL	0.09727 mL	0.30000 mL	3.706	-0.00719	0.81084	0.00039	10.0 s
39:30.1	Data point 39	1.50000 mL	0.10212 mL	0.09875 mL	0.30000 mL	3.908	-0.01381	0.88552	0.00072	10.5 s
40:06.1	Data point 40	1.50000 mL	0.10212 mL	0.09986 mL	0.30000 mL	4.220	-0.00595	0.67659	0.00036	10.0 s
40:51.7	Data point 41	1.50000 mL	0.10212 mL	0.10045 mL	0.30000 mL	4.415	-0.00682	0.73657	0.00039	10.5 s
41:38.0	Data point 42	1.50000 mL	0.10212 mL	0.10087 mL	0.30000 mL	4.612	-0.01104	0.72091	0.00064	10.5 s
42:29.5	Data point 43	1.50000 mL	0.10212 mL	0.10118 mL	0.30000 mL	4.814	-0.01440	0.75675	0.00082	10.5 s
43:05.4	Data point 44	1.50000 mL	0.10212 mL	0.10141 mL	0.30000 mL	5.068	-0.01600	0.81524	0.00088	11.5 s
43:47.3	Data point 45	1.50000 mL	0.10212 mL	0.10158 mL	0.30000 mL	5.325	-0.01213	0.64755	0.00074	12.0 s
44:30.0	Data point 46	1.50000 mL	0.10212 mL	0.10174 mL	0.30000 mL	5.861	-0.01983	0.98013	0.00099	35.5 s
45:36.0	Data point 47	1.50000 mL	0.10212 mL	0.10181 mL	0.30000 mL	6.309	-0.01961	0.97472	0.00098	56.0 s
47:02.6	Data point 48	1.50000 mL	0.10212 mL	0.10186 mL	0.30000 mL	6.639	-0.03066	0.99363	0.00152	Timed out at 59.5 s
48:28.0	Data point 49	1.50000 mL	0.10212 mL	0.10191 mL	0.30000 mL	7.034	-0.05072	0.99593	0.00251	Timed out at 59.5 s
49:58.5	Data point 50	1.50000 mL	0.10212 mL	0.10195 mL	0.30000 mL	7.398	-0.06220	0.99680	0.00308	Timed out at 59.5 s
51:29.0	Data point 51	1.50000 mL	0.10212 mL	0.10200 mL	0.30000 mL	7.885	-0.06202	0.99692	0.00307	Timed out at 59.5 s
52:59.4	Data point 52	1.50000 mL	0.10212 mL	0.10205 mL	0.30000 mL	8.135	-0.04192	0.98906	0.00208	Timed out at 59.5 s
54:30.0	Data point 53	1.50000 mL	0.10212 mL	0.10209 mL	0.30000 mL	8.402	-0.02237	0.99033	0.00111	Timed out at 59.5 s
56:00.4	Data point 54	1.50000 mL	0.10212 mL	0.10214 mL	0.30000 mL	8.573	-0.01945	0.95229	0.00098	53.5 s
57:24.5	Data point 55	1.50000 mL	0.10212 mL	0.10221 mL	0.30000 mL	8.793	-0.01809	0.98417	0.00090	34.5 s
58:39.9	Data point 56	1.50000 mL	0.10212 mL	0.10230 mL	0.30000 mL	9.005	-0.01939	0.93292	0.00099	19.5 s
1:00:24.9	Data point 57	1.50000 mL	0.16011 mL	0.10230 mL	0.80000 mL	1.959	-0.01114	0.87304	0.00059	10.0 s
1:01:11.2	Data point 58	1.50000 mL	0.16011 mL	0.12105 mL	0.80000 mL	2.170	0.00081	0.04813	0.00018	10.0 s
1:01:46.9	Data point 59	1.50000 mL	0.16011 mL	0.13271 mL	0.80000 mL	2.378	0.00136	0.09971	0.00021	10.0 s
1:02:22.5	Data point 60	1.50000 mL	0.16011 mL	0.14017 mL	0.80000 mL	2.585	0.01209	0.68746	0.00072	10.0 s
1:02:58.1	Data point 61	1.50000 mL	0.16011 mL	0.14513 mL	0.80000 mL	2.787	0.00716	0.56892	0.00047	10.0 s
1:03:33.6	Data point 62	1.50000 mL	0.16011 mL	0.14866 mL	0.80000 mL	2.998	-0.00487	0.59781	0.00031	10.0 s
1:04:09.0	Data point 63	1.50000 mL	0.16011 mL	0.15129 mL	0.80000 mL	3.171	0.00223	0.08135	0.00039	10.0 s
1:04:54.7	Data point 64	1.50000 mL	0.16011 mL	0.15376 mL	0.80000 mL	3.364	-0.00945	0.67088	0.00057	10.0 s
1:05:40.5	Data point 65	1.50000 mL	0.16011 mL	0.15555 mL	0.80000 mL	3.553	-0.00773	0.66839	0.00047	10.0 s



Assay Events

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09016**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:06:16.0	Data point 66	1.50000 mL	0.16011 mL	0.15691 mL	0.80000 mL	3.758	-0.00478	0.09544	0.00076	10.0 s
1:06:51.4	Data point 67	1.50000 mL	0.16011 mL	0.15793 mL	0.80000 mL	3.973	0.00088	0.00414	0.00068	10.0 s
1:07:26.8	Data point 68	1.50000 mL	0.16011 mL	0.15863 mL	0.80000 mL	4.186	-0.01639	0.67438	0.00099	10.0 s
1:08:02.3	Data point 69	1.50000 mL	0.16011 mL	0.15912 mL	0.80000 mL	4.378	-0.01336	0.45806	0.00098	10.0 s
1:08:37.7	Data point 70	1.50000 mL	0.16011 mL	0.15945 mL	0.80000 mL	4.589	-0.00985	0.60220	0.00063	11.0 s
1:09:14.1	Data point 71	1.50000 mL	0.16011 mL	0.15967 mL	0.80000 mL	4.736	-0.00475	0.10626	0.00072	11.5 s
1:09:56.1	Data point 72	1.50000 mL	0.16011 mL	0.15995 mL	0.80000 mL	5.134	-0.01189	0.37022	0.00096	12.0 s
1:10:43.8	Data point 73	1.50000 mL	0.16011 mL	0.16009 mL	0.80000 mL	5.393	-0.01905	0.93142	0.00098	34.5 s
1:11:48.9	Data point 74	1.50000 mL	0.16011 mL	0.16018 mL	0.80000 mL	5.755	-0.01516	0.77806	0.00085	45.5 s
1:13:05.0	Data point 75	1.50000 mL	0.16011 mL	0.16025 mL	0.80000 mL	6.047	-0.01855	0.94284	0.00094	50.5 s
1:14:26.2	Data point 76	1.50000 mL	0.16011 mL	0.16030 mL	0.80000 mL	6.272	-0.01969	0.96730	0.00099	58.0 s
1:15:49.6	Data point 77	1.50000 mL	0.16011 mL	0.16035 mL	0.80000 mL	6.474	-0.02760	0.99228	0.00137	Timed out at 59.5 s
1:17:20.1	Data point 78	1.50000 mL	0.16011 mL	0.16040 mL	0.80000 mL	6.897	-0.06395	0.99250	0.00317	Timed out at 59.5 s
1:18:45.5	Data point 79	1.50000 mL	0.16011 mL	0.16044 mL	0.80000 mL	7.185	-0.06453	0.99687	0.00319	Timed out at 59.5 s
1:20:16.1	Data point 80	1.50000 mL	0.16011 mL	0.16049 mL	0.80000 mL	7.570	-0.08020	0.98798	0.00398	Timed out at 59.5 s
1:21:46.6	Data point 81	1.50000 mL	0.16011 mL	0.16054 mL	0.80000 mL	7.910	-0.05115	0.99413	0.00253	Timed out at 59.5 s
1:23:17.1	Data point 82	1.50000 mL	0.16011 mL	0.16058 mL	0.80000 mL	8.105	-0.04177	0.93249	0.00214	Timed out at 59.5 s
1:24:52.7	Data point 83	1.50000 mL	0.16011 mL	0.16065 mL	0.80000 mL	8.398	-0.02637	0.89962	0.00137	Timed out at 59.5 s
1:26:33.5	Data point 84	1.50000 mL	0.16011 mL	0.16075 mL	0.80000 mL	8.655	-0.01834	0.88375	0.00096	28.0 s
1:27:37.2	Data point 85	1.50000 mL	0.16011 mL	0.16084 mL	0.80000 mL	8.817	-0.01433	0.54002	0.00096	16.5 s
1:28:29.4	Data point 86	1.50000 mL	0.16011 mL	0.16096 mL	0.80000 mL	9.030	-0.01224	0.37247	0.00099	14.0 s
1:28:52.4	Assay volumes	1.50000 mL	0.16011 mL	0.16096 mL	0.80000 mL					

Sample name: **M18_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.100 mL			
Partition solvent added	Manual in advance			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	60 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M18_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.500 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.102	3/9/2018 11:02:43 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus S	0.9967	3/9/2018 11:02:43 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jH	1.2	3/9/2018 11:02:43 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jOH	0.0	3/9/2018 11:02:43 PM	C:\Sirius_T3\HCl18C09.t3r
Base concentration factor	1.000	3/9/2018 11:02:44 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	1.000	3/9/2018 11:02:44 PM	C:\Sirius_T3\HCl18C09.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 11:05:59 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 11:27:22 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 11:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 10:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M18_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09016**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 10:59:35 AM
Titration		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+4.01 mV		3/9/2018 11:03:12 PM
Filling solution	3M KCl	KCL097	3/9/2018 11:05:42 AM
Liquids			
Wash 1	50% IPA:50% Water		3/9/2018 11:04:22 AM
Wash 2	0.5% Triton X-100 in H2O		3/9/2018 11:04:25 AM
Buffer position 1	pH7 Wash		3/9/2018 11:04:27 AM
Buffer position 2	pH 7		3/9/2018 11:04:30 AM
Storage position			3/9/2018 11:05:04 AM
Wash water	5e+003 mL	02-27-2018	2/27/2018 10:54:39 AM
Waste	1.1e+004 mL		11/28/2017 11:36:29 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	123:16:41		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		



Assay Settings

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09016**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09016_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 11:02:44 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00